WHAT IS CLAIMED IS:

1. A method of deriving data regarding a fragment molecule that is under evaluation regarding its interaction with a protein, the method comprising:
   (a) identifying conformers of the fragment;
   (b) selecting conformers that are representative of clusters of the identified conformers; and
   (c) performing the *ab initio* or semi-empirical calculation and analysis on the selected conformer.

2. The method of claim 1, further comprising:
   (a) for each atom of the selected conformer, determining an atom type.

3. The method of claim 1, further comprising:
   (a) symmetrizing the selected conformer if symmetry is recognized.

4. The method of claim 1, further comprising:
   (a) calculating a fragment-fragment cutoff for the selected conformer.

5. The method of claim 1, further comprising:
   (a) calculating a solvation energy for the selected conformer.

6. The method of claim 1, further comprising:
   (a) calculating an energy offset for the selected conformer.

7. The method of claim 1, further comprising:

(a) determining a derivatization point of the selected conformer; and

(b) assigning a score to the derivatization point indicative of the ease of bonding at the derivatization point.

8. The method of claim 1, further comprising:

(a) assigning the selected conformer to a category.

9. The method of claim 1, further comprising:

(a) assigning a name to the selected conformer.

10. The method of claim 1, further comprising:

(a) storing data derived in steps (a) through (m) in a database.

11. The method of claim 1, wherein said step (b) comprises performing force field calculations based on one or more force field models.

12. The method of claim 1, wherein said step (c) comprises performing conformational searches of the fragment and identifying relevant conformations of a fragment.

13. The method of claim 1, wherein said step (d) comprises performing cluster analysis of the relevant conformations identified in step (6) and selecting the representative conformation or conformations in the identified clusters.

14. The method of claim 1, wherein said step (f) comprises:

(i) receiving (x,y,z) coordinates of the initial three-dimensional model of the selected conformer;

(ii) determining structure of the selected conformer at an electron level of detail;

(iii) performing *ab initio* analysis of the electron-level structure of the selected conformer;

(iv) performing charge calculations on the electron-level structure; and

(v) refining the initial three-dimensional model on the basis of the *ab initio* analysis and the charge calculations.

15. The method of claim 1, wherein said step (g) comprises:

(i) determining the element of the atom; and

(ii) mapping the atom to a type based on the element, any structures to which the atom is bonded, and hybridization.

16. The method of claim 1, wherein said step (h) comprises:

(i) recognizing if symmetry is present in the selected conformer;

(ii) if so, comparing corresponding bond lengths; and

(iii) if a difference is found in the corresponding bond lengths, and if the difference is below a threshold value, adjusting the corresponding bond lengths.

17. The method of claim 16, wherein said step (iii) comprises:

averaging the corresponding bond lengths to produce an average bond length; and

replacing each corresponding bond length with the average bond length.

18. The method of claim 1, wherein said step (h) comprises:

(i) recognizing if symmetry is present in the selected conformer;

(ii) if so, comparing a pair of corresponding bond angles; and

(iii) if a difference is found in bond angles, and if the difference is above a threshold value, adjusting the corresponding bond angles.

19. The method of claim 18, wherein said step (iii) comprises:

averaging the corresponding bond angles to produce an average bond angle, and

replacing each corresponding bond angle with the average bond angle.

20. The method of claim 1, wherein said step (h) comprises:

(i) Recognizing if symmetry is present in the selected conformer;

(ii) If so, comparing a pair of corresponding partial charges on symmetrical atoms; and

(iii) if a difference is found in the partial charges on symmetrical atoms, and if the difference is greater than a threshold value, adjusting the partial charges of the corresponding symmetrical atoms.

21. The method of claim 20, wherein said step (iii) comprises:

averaging the corresponding partial charges of the atoms to produce an average partial charge for the atoms, and

replacing each corresponding partial charge with the average partial charge.

22. The method of claim 1, wherein said step (i) comprises:

determining a center point of the selected conformer;

determining the size of the smallest sphere that could encompass the selected conformer while centered at the center point; and

defining a fragment-fragment cutoff value for the selected conformer to be the diameter of the sphere.

23. The method of claim 22, wherein the center point is the center of mass of the selected conformer.

24. The method of claim 22, wherein the center point is the geometric center of the selected conformer.

25. A method of deriving data regarding a fragment molecule that is under evaluation regarding its interaction with a protein, comprising calculating an energy offset for said fragment molecule.